Physics of the Solid State 2013 vol.55 N12, pages 2558-2565

Changes in the structure of the Rb2NaYF6: Yb3+ crystal upon transition from the cubic to tetragonal phase

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Abstract

The pattern of lattice distortions occurring in the vicinity of Yb3+ ions during the transition of the Rb2NaYF6: Yb3+ crystal from the cubic to tetragonal phase has been revealed using all the parameters of the empirically found crystal fields for paramagnetic centers of the Yb3+ ions with cubic and tetragonal symmetry. It has been shown that the YbF6 octahedra are rotated about the fourfold axis through an angle approximately equal to 1.2°. Moreover, the octahedra themselves are deformed so that the F- ions symmetrically located in the plane perpendicular to the axis of rotation come close to the impurity ion at a distance of 0.0004 nm. The fluoride ions located on the axis of rotation, conversely, move away from the Yb3+ ion at a distance of 0.0005 nm. Based on the obtained results, it has been concluded that the total condensate of order parameters of the studied phase transition involves not only the critical rotations of octahedral groups but also the noncritical displacements of atoms in the rotated octahedra.

http://dx.doi.org/10.1134/S1063783413120214